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ANNOUNCEMENT TO AUTHORS

PUBLICATION OF X-RAY CRYSTALLOGRAPHIC WORK IN TETRAHEDRON LETTERS

A major problem associated with the publication of preliminary reports of crystallographic work is the non-availability to interested readers of the atomic co-ordinates associated with the work. Although in the normal course of events such data would be expected to appear in the follow-up paper, many cases occur where the period between publication of the preliminary report and the substantive paper is many years or the full paper never appears in print. After consultation with the Cambridge Crystallographic Data Centre (CCDC) the Editors have resolved to press authors of preliminary reports of X-ray crystallographic work to submit together with their communication certain material for deposition with the Centre. This material will be checked at the Centre for internal consistency and, afterwards, will be available on request to interested readers. The procedure to be adopted is similar to that already in use for *Chemical Communications* and will be as follows:

(i) In addition to the communication and the customary covering letter of justification, the authors will be expected to provide a complete list of refined co-ordinates and a table of bond distances unless these are given in full in the manuscript. Direct computer output is preferred. A print program should be used which yields concise tables. The contents of the tables should be non-redundant and readily interpretable. If these guidelines cannot be satisfied then the author should present manually-typed tables. If the complete "crystal data" (i.e. cell dimensions and standard deviations, space group, number Z of formula units per cell) are not listed in the manuscript, these must also be submitted.

It should be emphasized that the co-ordinates submitted for deposition, whilst not necessarily being "fully" refined, should correspond to the stage of refinement described in the preliminary communication and should be the set for which the R factor is quoted. It follows that all bond distances given in the preliminary communication should correspond, apart from any rounding-off errors, with bond distances which can be calculated from the deposited co-ordinates.

(ii) The communication will be assessed in the customary fashion, the material for deposition also being made available to the referees concerned. If the communication is accepted the Editors will forward the material for deposition to the CCDC.

(iii) The CCDC will acknowledge receipt of the material. When a communication is published the deposited material will be evaluated and included in their files as part of their normal abstracting cycle. The evaluation consists of recalculation of the bond lengths from the author's co-ordinates and comparison of these with the author's values. All data on the Centre's files have to pass this internal consistency test. It will not, however, be possible for the evaluation to be made before the appearance of the preliminary communication in print.

(iv) Finally, where an author plans not to follow-up his preliminary communication with a full paper he will be required to submit, in addition to the material outlined above, a copy of the structure factor table for the work presented for deposition with the British Library, Lending Division. In this way, it too will be available to interested readers.

(v) The typescript for publication in *Tetrahedron Letters* should include the following footnote(s) referring to the deposited data:

(a) The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK. Any request should be accompanied by the full literature citation for this communication.

(b) Supplementary data available [insert brief details], structure factors. See Announcement to Authors, *Tetrahedron Letters*, 47,5154 (1983).